Susan B Sinnott

List of Publications by Year
in descending order

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281 papers	14,723 citations	23500 58 h-index	22764 112 g-index
290 all docs	290 docs citations	290 times ranked	13632 citing authors

#	Article	IF	Citations
1	A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons. Journal of Physics Condensed Matter, 2002, 14, 783-802.	0.7	2,826
2	Model of carbon nanotube growth through chemical vapor deposition. Chemical Physics Letters, 1999, 315, 25-30.	1.2	515
3	Carbon Nanotubes: Synthesis, Properties, and Applications. Critical Reviews in Solid State and Materials Sciences, 2001, 26, 145-249.	6.8	403
4	Effect of chemical functionalization on the mechanical properties of carbon nanotubes. Chemical Physics Letters, 1998, 295, 273-278.	1.2	305
5	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. Physical Review Letters, 2017, 118, 106101.	2.9	262
6	Chemical Functionalization of Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2002, 2, 113-123.	0.9	242
7	Parametrization of a reactive many-body potential for Moâ€“S systems. Physical Review B, 2009, 79, .	1.1	241
8	Classical atomistic simulations of surfaces and heterogeneous interfaces with the charge-optimized many body (COMB) potentials. Materials Science and Engineering Reports, 2013, 74, 255-279.	14.8	222
9	Compression of Carbon Nanotubes Filled withC60,CH4, or Ne: Predictions from Molecular Dynamics Simulations. Physical Review Letters, 2002, 88, 205505.	2.9	204
10	A Computational Study of Molecular Diffusion and Dynamic Flow through Carbon Nanotubes. Journal of Physical Chemistry B, 2000, 104, 4618-4624.	1.2	197
11	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. Journal of Physical Chemistry C, 2016, 120, 3550-3556.	1.5	196
12	Reactive Potentials for Advanced Atomistic Simulations. Annual Review of Materials Research, 2013, 43, 109-129.	4.3	184
13	Mechanical properties of nanotubule fibers and composites determined from theoretical calculations and simulations. Carbon, 1998, 36, 1-9.	5.4	183
14	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. Nano Letters, 2017, 17, 5251-5257.	4.5	172
15	Molecular dynamics simulations of the filling and decorating of carbon nanotubules. Nanotechnology, 1999, 10, 273-277.	1.3	166
16	Charge optimized many-body potential for theSiâ•SiO2system. Physical Review B, 2007, 75, .	1.1	159
17	Ceramic/metal interface structures and their relationship to atomic- and meso-scale properties. Materials Science and Engineering Reports, 2003, 43, 1-59.	14.8	155
18	Separation of Organic Molecular Mixtures in Carbon Nanotubes and Bundles:â€‰ Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2001, 105, 6916-6924.	1.2	147

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19	Mixed Bloch-NÃ©el-Ising character of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>180</mml:mn><mml:mo>Â°</mml:mo></mml:mrow></mml:math>ferroelectric domain walls. Physical Review B, 2009, 80, .	1.1	146
20	Frictional anisotropy of oriented carbon nanotube surfaces. Tribology Letters, 2005, 18, 59-62.	1.2	136
21	Interactions of Carbon-Nanotubule Proximal Probe Tips with Diamond and Graphene. Physical Review Letters, 1998, 81, 2260-2263.	2.9	131
22	Charge-optimized many-body potential for the hafnium/hafnium oxide system. Physical Review B, 2010, 81, .	1.1	130
23	Behavior of molecules and molecular ions near a field emitter. New Journal of Physics, 2016, 18, 033031.	1.2	130
24	Energetics of intrinsic point defects in uranium dioxide from electronic-structure calculations. Journal of Nuclear Materials, 2009, 384, 61-69.	1.3	127
25	Density functional study of the bonding in small silicon clusters. Journal of Chemical Physics, 1992, 97, 4149-4161.	1.2	121
26	Prediction of high-temperature point defect formation in TiO2 from combined ab initio and thermodynamic calculations. Acta Materialia, 2007, 55, 4325-4337.	3.8	120
27	Carbon doping of WS ₂ monolayers: Bandgap reduction and p-type doping transport. Science Advances, 2019, 5, eaav5003.	4.7	119
28	A Combined Computational and Experimental Study of Ion-Beam Modification of Carbon Nanotube Bundles. Journal of Physical Chemistry B, 2001, 105, 12719-12725.	1.2	112
29	Molecular Dynamics Simulation Study of Carbon Nanotube Welding under Electron Beam Irradiation. Nano Letters, 2004, 4, 109-114.	4.5	112
30	Stability of intrinsic defects and defect clusters in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Li</mml:mi><mml:mi mathvariant="normal">Nb</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>from density functional theory calculations. Physical Review B, 2008, 78, .	1.1	109
31	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>	1.1	106
32	The growth and modification of materials via ionâ€“surface processing. Surface Science, 2002, 500, 500-522.	0.8	103
33	Tribological properties of carbon nanotube bundles predicted from atomistic simulations. Surface Science, 2001, 487, 87-96.	0.8	102
34	Ion separation using a Y-junction carbon nanotube. Nanotechnology, 2006, 17, 895-900.	1.3	96
35	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. Computational Materials Science, 2016, 122, 183-190.	1.4	95
36	Computational Study of Low Interlayer Friction in Ti_{n+1}C_n (n = 1, 2, and 3) MXene. ACS Applied Materials & Interfaces, 2017, 9, 34467-34479.	4.0	93

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37	A reactive empirical bond order (REBO) potential for hydrocarbonâ€“oxygen interactions. Journal of Physics Condensed Matter, 2004, 16, 7261-7275.	0.7	91
38	Variable Charge Reactive Potential for Hydrocarbons to Simulate Organic-Copper Interactions. Journal of Physical Chemistry A, 2012, 116, 7976-7991.	1.1	91
39	Second-generation charge-optimized many-body potential for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow></mml:msub></mml:mrow></mml:math> amorphous silica. Physical Review B, 2010, 82, .	1.1	89
40	Multiscale computational understanding and growth of 2D materials: a review. Npj Computational Materials, 2020, 6, .	3.5	89
41	Thermal transport properties of uranium dioxide by molecular dynamics simulations. Journal of Nuclear Materials, 2008, 375, 388-396.	1.3	87
42	Corrected effective-medium study of metal-surface relaxation. Physical Review B, 1991, 44, 8927-8941.	1.1	85
43	Chemical functionalization of carbon nanotubes through energetic radical collisions. Physical Review B, 2000, 61, R16343-R16346.	1.1	85
44	Sorption of Butane on Carbon Multiwall Nanotubes at Room Temperature. Langmuir, 2001, 17, 7540-7544.	1.6	85
45	Multi-Step Topochemical Pathway to Metastable Mo₂AlB₂ and Related Two-Dimensional Nanosheet Heterostructures. Journal of the American Chemical Society, 2019, 141, 10852-10861.	6.6	84
46	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. Applied Physics Letters, 2016, 108, .	1.5	79
47	Grain Boundaries in Uranium Dioxide: Scanning Electron Microscopy Experiments and Atomistic Simulations. Journal of the American Ceramic Society, 2011, 94, 1893-1900.	1.9	78
48	Elastic torsional responses of carbon nanotube systems. Journal of Applied Physics, 2007, 101, 084309.	1.1	76
49	Effect of polyatomic ion structure on thin-film growth: Experiments and molecular dynamics simulations. Journal of Applied Physics, 2000, 88, 5004-5016.	1.1	75
50	Friction Properties of Carbon Nano-Onions from Experiment and Computer Simulations. Tribology Letters, 2010, 37, 75-81.	1.2	75
51	Computational discovery of stable<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2016, 94, .	1.1	75
52	Transition from Thermal to Athermal Friction under Cryogenic Conditions. Physical Review Letters, 2009, 102, 186102.	2.9	73
53	Tensile mechanical behavior of hollow and filled carbon nanotubes under tension or combined tension-torsion. Applied Physics Letters, 2007, 90, 023102.	1.5	72
54	Defect Engineering of BiI₃ Single Crystals: Enhanced Electrical and Radiation Performance for Room Temperature Gamma-Ray Detection. Journal of Physical Chemistry C, 2014, 118, 3244-3250.	1.5	72

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55	Atomistic simulations of copper oxidation and Cu/Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O interfaces using charge-optimized many-body potentials. Physical Review B, 2011, 84, .	1.1	68
56	Development of a ReaxFF Reactive Force Field for NaSiO_x/Water Systems and Its Application to Sodium and Proton Self-Diffusion. Journal of Physical Chemistry C, 2018, 122, 19613-19624.	1.5	63
57	Computational discovery and characterization of polymorphic two-dimensional IVâ€“V materials. Applied Physics Letters, 2016, 109, .	1.5	60
58	Variable charge many-body interatomic potentials. MRS Bulletin, 2012, 37, 504-512.	1.7	58
59	Effects of unique ion chemistry on thin-film growth by plasma-surface interactions. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 23-27.	3.3	57
60	Energetics of Oxidation in MoS₂Nanoparticles by Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 10606-10616.	1.5	55
61	Sliding orientation effects on the tribological properties of polytetrafluoroethylene. Journal of Applied Physics, 2007, 102, .	1.1	54
62	Nanoindentation of gold and gold alloys by molecular dynamics simulation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 651, 346-357.	2.6	54
63	Predictions of a Spiral Diffusion Path for Nonspherical Organic Molecules in Carbon Nanotubes. Physical Review Letters, 2002, 89, 278301.	2.9	53
64	Molecular dynamics simulations of electron and ion beam irradiation of multiwalled carbon nanotubes: The effects on failure by inner tube sliding. Physical Review B, 2006, 73, .	1.1	52
65	Thermodynamics of fission products in UO_{2 Â±x}. Journal of Physics Condensed Matter, 2009, 21, 435602.	0.7	52
66	Atomistic simulations of the nanometer-scale indentation of amorphous-carbon thin films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1997, 15, 936-940.	0.9	51
67	Segregation of xenon to dislocations and grain boundaries in uranium dioxide. Physical Review B, 2011, 84, .	1.1	49
68	Structure and energetics of 180Â° domain walls in PbTiO₃by density functional theory. Journal of Physics Condensed Matter, 2011, 23, 175902.	0.7	48
69	Critical assessment of UO2 classical potentials for thermal conductivity calculations. Journal of Materials Science, 2012, 47, 7693-7702.	1.7	48
70	Thermal Transport in Offâ€Stoichiometric Uranium Dioxide by Atomic Level Simulation. Journal of the American Ceramic Society, 2009, 92, 850-856.	1.9	47
71	Molecular dynamics study of the adhesion of Cu/SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>interfaces using a variable-charge interatomic potential. Physical Review B, 2011, 83, .	1.1	47
72	Vacancyâ€Ordered Structure of Cubic Bismuth Oxide from Simulation and Crystallographic Analysis. Journal of the American Ceramic Society, 2008, 91, 2349-2356.	1.9	45

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73	Molecular dynamics of carbon nanotubule proximal probe tip-surface contacts. Physical Review B, 1999, 60, 13786-13791.	1.1	44
74	Three decades of many-body potentials in materials research. MRS Bulletin, 2012, 37, 469-473.	1.7	44
75	Lubrication mechanisms of hollow-core inorganic fullerene-like nanoparticles: coupling experimental and computational works. Nanotechnology, 2012, 23, 375701.	1.3	44
76	Fitting empirical potentials: Challenges and methodologies. Current Opinion in Solid State and Materials Science, 2013, 17, 263-270.	5.6	44
77	Effects of edge dislocations on thermal transport in UO2. Journal of Nuclear Materials, 2013, 434, 203-209.	1.3	44
78	Modification of carbon nanotube-polystyrene matrix composites through polyatomic-ion beam deposition predictions from molecular dynamics simulations. Composites Science and Technology, 2003, 63, 1663-1669.	3.8	42
79	A critical assessment of interatomic potentials for ceria with application to its elastic properties. Solid State Ionics, 2010, 181, 551-556.	1.3	42
80	Constant temperature molecular dynamics simulations of energetic particleâ€“solid collisions: comparison of temperature control methods. Journal of Computational Physics, 2004, 200, 251-266.	1.9	41
81	Stability and charge transfer levels of extrinsic defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiNbO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2010, 82, .	1.1	41
82	Equilibrium and Nonequilibrium Transport of Oxygen in Carbon Nanotubes. Nano Letters, 2005, 5, 793-798.	4.5	40
83	Predicted mechanical properties of a coiled carbon nanotube. Carbon, 2012, 50, 968-976.	5.4	40
84	Structure and diffusion of intrinsic defect complexes in LiNbO₃from density functional theory calculations. Journal of Physics Condensed Matter, 2010, 22, 135002.	0.7	39
85	Molecular dynamics investigation of the lubrication mechanism of carbon nano-onions. Computational Materials Science, 2012, 54, 91-96.	1.4	39
86	Simulated engineering of nanostructures. Nanotechnology, 1996, 7, 161-167.	1.3	38
87	Torsional stiffening of carbon nanotube systems. Applied Physics Letters, 2007, 91, .	1.5	38
88	Mechanical behavior of MoS2 nanotubes under compression, tension, and torsion from molecular dynamics simulations. Journal of Applied Physics, 2012, 112, .	1.1	38
89	Effect of Temperature on the Friction and Wear of PTFE by Atomic-Level Simulation. Tribology Letters, 2015, 58, 1.	1.2	38
90	Grapheneâ€“Titanium Interfaces from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 33288-33297.	4.0	37

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91	Surface patterning by atomically-controlled chemical forces: molecular dynamics simulations. Surface Science, 1994, 316, L1055-L1060.	0.8	36
92	Ab Initio Calculations of Intrinsic Defects in Rutile TiO2. Journal of the American Ceramic Society, 2005, 88, 737-741.	1.9	35
93	Structure and energetics of Er defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiNbO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> first-principles and thermodynamic calculations. Physical Review B, 2009, 80, .	1.1	35
94	Reparameterization of the REBO-CHO potential for graphene oxide molecular dynamics simulations. Physical Review B, 2011, 84, .	1.1	35
95	Ab Initio Calculations of Pristine and Doped Zirconia Î£5 (310)/[001] Tilt Grain Boundaries. Journal of the American Ceramic Society, 2002, 85, 1594-1600.	1.9	34
96	Simulating Multifunctional Structures. Science, 2009, 325, 1634-1635.	6.0	34
97	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. Journal of Physical Chemistry C, 2019, 123, 3180-3187.	1.5	34
98	Computational Studies of Non-Equilibrium Molecular Transport through Carbon Nanotubes. Journal of Physical Chemistry B, 2004, 108, 9861-9870.	1.2	33
99	Molecular Dynamics Simulations of the Chemical Modification of Polystyrene through CxFy+Beam Deposition. Journal of Physical Chemistry B, 2004, 108, 18993-19001.	1.2	33
100	Morphology and Mechanical Properties of Surfactant Aggregates at Waterâ^'Silica Interfaces:Â Molecular Dynamics Simulations. Langmuir, 2005, 21, 5337-5342.	1.6	33
101	Effect of the sliding orientation on the tribological properties of polyethylene in molecular dynamics simulations. Journal of Applied Physics, 2008, 103, 083502.	1.1	33
102	Piecewise-stationary bandit problems with side observations. , 2009, , .		33
103	Stoichiometry of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">LaFeO</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> surface determined from first-principles and thermodynamic calculations. Physical Review B, 2011, 83, .	1.1	33
104	Polymerization via Clusterâ^'Solid Surface Impacts:Â Molecular Dynamics Simulations. Journal of Physical Chemistry B, 1997, 101, 6883-6890.	1.2	32
105	Energetics of charged point defects in rutile TiO2 by density functional theory. Acta Materialia, 2009, 57, 5882-5891.	3.8	32
106	Three-dimensional atomic scale electron density reconstruction of octahedral tilt epitaxy in functional perovskites. Nature Communications, 2018, 9, 5220.	5.8	32
107	Molecular dynamics simulations of polyatomic-ion beam deposition-induced chemical modification of carbon nanotube/polymer composites. Journal of Materials Chemistry, 2004, 14, 719.	6.7	31
108	Comparison of morphology and mechanical properties of surfactant aggregates at waterâ€“silica and waterâ€“graphite interfaces from molecular dynamics simulations. Journal of Colloid and Interface Science, 2006, 296, 342-349.	5.0	31

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109	NSF cyberinfrastructures: A new paradigm for advancing materials simulation. Current Opinion in Solid State and Materials Science, 2013, 17, 298-304.	5.6	31
110	An ab initio investigation of the effect of alloying elements on the elastic properties and magnetic behavior of Ni3Al. Computational Materials Science, 2015, 101, 39-46.	1.4	31
111	Molecular Simulation of Capture of Sulfur-Containing Gases by Porous Aromatic Frameworks. Journal of Physical Chemistry C, 2018, 122, 18456-18467.	1.5	31
112	Effect of Filling on the Compressibility of Carbon Nanotubes: Predictions from Molecular Dynamics Simulations. Journal of Nanoscience and Nanotechnology, 2005, 5, 536-541.	0.9	30
113	Combined computational and experimental study of Ar beam induced defect formation in graphite. Nuclear Instruments & Methods in Physics Research B, 2007, 262, 240-248.	0.6	30
114	Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities. Annual Review of Materials Research, 2007, 37, 239-270.	4.3	29
115	Mechanisms of Zr surface corrosion determined via molecular dynamics simulations with charge-optimized many-body (COMB) potentials. Journal of Nuclear Materials, 2014, 452, 285-295.	1.3	29
116	Nanostructure of Fluorocarbon Films Deposited on Polystyrene from Hyperthermal C3F5+ Ions. Journal of Physical Chemistry B, 2004, 108, 9656-9664.	1.2	28
117	The effect of normal load on polytetrafluoroethylene tribology. Journal of Physics Condensed Matter, 2009, 21, 144201.	0.7	28
118	Data-Driven Model for Estimation of Friction Coefficient Via Informatics Methods. Tribology Letters, 2012, 47, 211-221.	1.2	28
119	Nanoindentation of Zr by molecular dynamics simulation. Journal of Nuclear Materials, 2015, 467, 742-757.	1.3	28
120	Effect of pores and He bubbles on the thermal transport properties of UO2 by molecular dynamics simulation. Journal of Nuclear Materials, 2015, 456, 253-259.	1.3	28
121	Ab Initio Molecular Dynamics Study of Methanol Adsorption on Copper Clusters. Journal of Physical Chemistry A, 2007, 111, 441-449.	1.1	27
122	Effect of inversion on thermoelastic and thermal transport properties of MgAl2O4 spinel by atomistic simulation. Journal of Materials Science, 2011, 46, 55-62.	1.7	27
123	Atomistic simulations of the adsorption and migration barriers of Cu adatoms on ZnO surfaces using COMB potentials. Surface Science, 2012, 606, 1280-1288.	0.8	27
124	Growth and Structure of Cu and Au on the Nonpolar ZnO(101Ì…0) Surface: STM, XPS, and DFT Studies. Journal of Physical Chemistry C, 2013, 117, 18386-18397.	1.5	27
125	Effects of water on the mechanical properties of silica glass using molecular dynamics. Acta Materialia, 2019, 178, 36-44.	3.8	27
126	Investigation of the Influence of Thermostat Configurations on the Mechanical Properties of Carbon Nanotubes in Molecular Dynamics Simulations. Journal of Nanoscience and Nanotechnology, 2007, 7, 1518-1524.	0.9	26

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127	Probing the accuracy of reactive and non-reactive force fields to describe physical and chemical properties of graphene-oxide. Computational Materials Science, 2016, 114, 236-243.	1.4	26
128	Effect of ionic polarizability on oxygen diffusion in Î´-Bi2O3 from atomistic simulation. Ionics, 2010, 16, 297-303.	1.2	25
129	Influence of the Molecular Level Structure of Polyethylene and Polytetrafluoroethylene on Their Tribological Response. Tribology Letters, 2011, 42, 193-201.	1.2	25
130	Deformation processes in polycrystalline Zr by molecular dynamics simulations. Journal of Nuclear Materials, 2015, 462, 147-159.	1.3	25
131	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25
132	Effect of molecular interactions on carbon nanotube friction. Journal of Applied Physics, 2007, 102, .	1.1	24
133	Molecular dynamics simulations of CO2 reduction on Cu(111) and Cu/ZnO(10 <mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	1.6	24
134	Ab initiocalculations of rigid-body displacements at the Î£5 (210) tilt grain boundary inTiO2. Physical Review B, 2000, 61, 15645-15648.	1.1	23
135	Classical interatomic potential for orthorhombic uranium. Journal of Physics Condensed Matter, 2012, 24, 235403.	0.7	23
136	Charge-optimized many-body (COMB) potential for zirconium. Journal of Nuclear Materials, 2013, 441, 274-279.	1.3	23
137	Mapping Chemical Selection Pathways for Designing Multicomponent Alloys: an informatics framework for materials design. Scientific Reports, 2015, 5, 17960.	1.6	23
138	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	1.4	23
139	Ar beam modification of nanotube based composites using molecular dynamics simulations. Composites Science and Technology, 2008, 68, 2049-2055.	3.8	22
140	Intrinsic electrostatic effects in nanostructured ceramics. Physical Review B, 2010, 81, .	1.1	22
141	Tuning the torsional properties of carbon nanotube systems with axial prestress. Applied Physics Letters, 2008, 92, 253114.	1.5	21
142	Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design. Journal of Physical Chemistry C, 2014, 118, 20043-20069.	1.5	21
143	A charge optimized many-body (comb) potential for titanium and titania. Journal of Physics Condensed Matter, 2014, 26, 315007.	0.7	21
144	Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad. Computational Materials Science, 2018, 148, 231-241.	1.4	21

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145	Computational and experimental studies of phase separation in pentacene:C[sub 60] mixtures. Journal of Vacuum Science & Technology B, 2009, 27, 169.	1.3	20
146	Primary Radiation Defect Production in Polyethylene and Cellulose. Journal of Physical Chemistry B, 2012, 116, 13932-13938.	1.2	20
147	The role of charge and ionic radius on fission product segregation to a model UO2 grain boundary. Journal of Applied Physics, 2013, 113, .	1.1	20
148	Dataâ€driven glass/ceramic science research: Insights from the glass and ceramic and data science/informatics communities. Journal of the American Ceramic Society, 2019, 102, 6385-6406.	1.9	20
149	Preferred crystallographic orientation relationships of nickel films deposited on (100) cubic-zirconia substrates. Thin Solid Films, 2000, 372, 37-44.	0.8	19
150	Applied Potentials in Variable-Charge Reactive Force Fields for Electrochemical Systems. Journal of Physical Chemistry A, 2018, 122, 631-638.	1.1	19
151	Generation of 3D hydrocarbon thin films via organic molecular cluster collisions. Surface Science, 1998, 398, 195-202.	0.8	18
152	Stabilization Mechanisms of LaFeO3 (010) Surfaces Determined with First Principles Calculations. Journal of the American Ceramic Society, 2011, 94, 1931-1939.	1.9	18
153	Effect of surface reactivity on the nucleation of hydrocarbon thin films through molecular-cluster beam deposition. Surface Science, 1999, 426, 83-91.	0.8	17
154	Deflection of Nanotubes in Response to External Atomic Collisions. Nano Letters, 2005, 5, 263-268.	4.5	17
155	Structure of Î´-Bi2O3 from density functional theory: A systematic crystallographic analysis. Journal of Solid State Chemistry, 2009, 182, 1222-1228.	1.4	17
156	A charge-optimized many-body potential for the Uâ€“UO₂â€“O₂system. Journal of Physics Condensed Matter, 2013, 25, 505401.	0.7	17
157	Charge optimized many-body (COMB) potential for Al₂O₃materials, interfaces, and nanostructures. Journal of Physics Condensed Matter, 2015, 27, 305004.	0.7	17
158	Nanoindentation of ZrO2 and ZrO2/Zr systems by molecular dynamics simulation. Journal of Nuclear Materials, 2017, 486, 250-266.	1.3	17
159	Study of C3H5+ ion deposition on polystyrene and polyethylene surfaces using molecular dynamics simulations. Journal of Applied Physics, 2002, 92, 3363-3367.	1.1	16
160	Interaction of functionalized benzene molecules with carbon nanopores. Chemical Physics Letters, 2004, 389, 96-100.	1.2	16
161	Publisher's Note: Mixed Bloch-NÃ©el-Ising character of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>180</mml:mn><mml:mo>Â°</mml:mo></mml:mrow></mml:math>ferroelectric domain walls [Phys. Rev. B80, 060102 (2009)]. Physical Review B, 2009, 80, .	1.1	16
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